

# Remarks on BMV conjecture

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## Abstract

We show that for fixed  $A, B$ , hermitian nonnegative definite matrices, and fixed  $k$  the coefficients of the  $t^k$  in the polynomial  $\text{Tr}(A + tB)^m$  is positive if  $\text{Tr } AB > 0$  and  $m > N(A, B, k)$ .

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## 1 Introduction

It was shown by Lieb-Seiringer [4] that the Bessis-Moussa-Villani conjecture [1] to the following statement. Assume that  $A, B$   $n \times n$  are hermitian nonnegative definite matrices. Then the polynomial  $\text{Tr}(A + tB)^m$  has nonnegative Taylor coefficients. Note that  $\text{Tr } AB \geq 0$  and  $\text{Tr } AB = 0$  if and only if  $AB = 0$ . The aim of this paper to show the following asymptotic result. For a fixed integer  $k \geq 0$ , the coefficients of the  $t^k$  in the polynomial  $\text{Tr}(A + tB)^m$  is positive if  $\text{Tr } AB > 0$  and  $m > N(A, B, k)$ . We obtained this result in summer 2007. Since then another proof appeared in [2]. We also discuss the case of nonnegativity of all coefficients of  $t^3$  in  $\text{Tr}(A + tB)^m$  for  $n = 3$  and all  $m$ . I would like to thank to J. Borcea for drawing my attention to [2].

## 2 Preliminary results

Let  $\mathbb{C}^{m \times n}, H_n$  be the set of  $m \times n$  and  $n \times n$  hermitian matrices respectively. For  $A \in \mathbb{C}^{n \times n}$  let  $\text{Tr } A$  be the trace of  $A$ . Let  $A_1, \dots, A_k \in \mathbb{C}^{n \times n}$ . Then  $\text{Tr } A_1 \dots A_k$  is a cyclic invariant:

$$\text{Tr } A_1 A_2 \dots A_{k-1} A_k = \text{Tr } A_2 A_3 \dots A_k A_1 = \dots = \text{Tr } A_k A_1 \dots A_{k-1}.$$

Denote

$$(A + tB)^m = \sum_{i=0}^m t^i S_{m-i,i}(A, B), \quad A, B \in \mathbb{C}^{n \times n}. \quad (2.1)$$

Since

$$(A + tB)^{m+1} = (A + tB)(A + tB)^m = (A + tB)^m(A + tB)$$

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we deduce

$$\begin{aligned} S_{m+1,k}(A, B) &= AS_{m,k}(A, B) + BS_{m+1,k-1}(A, B) = \\ S_{m,k}(A, B)A + S_{m+1,k-1}(A, B)B, \quad m, k &= 0, 1, \dots, \end{aligned} \quad (2.2)$$

where we use the convention

$$S_{p,q}(A, B) = 0 \text{ if } \min(p, q) < 0. \quad (2.3)$$

Note that if  $A, B \in H_n$  are hermitian then  $S_{p,q}(A, B) \in H_n$  for each  $p, q \geq 0$ . For  $A \in H_n$  we denote by  $A \succ 0$ ,  $A \succeq 0$  the positive and the nonnegative definite matrices respectively.  $H_{n,+} := \{A \in H_n : A \succeq 0\}$ . The BMV conjecture is equivalent to  $\text{Tr} S_{p,q} \geq 0$  for each  $A, B \in H_{n,+}$ ,  $p, q \geq 0$ . [4]. Recall that  $\text{Tr} AB \geq 0$  if  $A, B \succeq 0$ . It is easy to show that  $\text{Tr} S_{p,q}(A, B) \neq 0$  if  $\min(p, q) \leq 2$ . (One uses the cyclic invariance of the trace and the fact  $\text{Tr} CD \geq 0$  if  $C, D \succeq 0$ ). By replacing the hermitian pair  $(A, B)$  with  $(UAU^*, UBU^*)$ , where  $U$  is a unitary matrix, without loss of generality we may assume that

$$A = \text{diag}(a_1, \dots, a_n), \quad a_1 \geq \dots \geq a_n \geq 0. \quad (2.4)$$

### 3 Asymptotic results

In view of the results of the results [3] it is of interest to consider the asymptotic behavior of  $\text{Tr} S_{m,k}(A, B)$  for a fixed  $A, B \in H_{n,+}$ ,  $k$  and  $m \rightarrow \infty$ .

**Theorem 3.1** *Let  $A, B \in H_{n,+}$ . If  $\text{Tr} AB = 0$  then  $AB = 0$ , Hence  $\text{Tr} S_{m,k}(A, B) = 0$  for any  $m, k \geq 1$ . Assume that  $\text{Tr} AB > 0$ . Let  $A$  be a diagonal matrix of the form (2.4) and  $B = [b_{ij}]_{i,j=1}^n$ . Let  $p \in \langle n \rangle$  be the smallest  $j$  such that  $a_j b_{jj} > 0$ . Then for each  $\epsilon > 0, k \in \mathbb{N}$  there exists  $N(A, B, \epsilon, k)$  such that*

$$\text{Tr} S_{m,k}(A, B) \geq (1 - \epsilon) b_{pp}^k a_p^m \binom{m+k}{k} \text{ for } m > N(A, B, \epsilon, k). \quad (3.1)$$

Furthermore, assume that  $a_p = \dots = a_{p+l-1} > a_{p+l}, l \in [1, n]$ . Denote by  $C = [b_{ij}]_{i,j=p}^{p+l-1} \in H_{l,+}$ . Then

$$\lim_{m \rightarrow \infty} \frac{\text{Tr} S_{m,k}(A, B)}{a_p^m \binom{m+k}{k}} = \text{Tr} C^k. \quad (3.2)$$

We prove this theorem using the following lemmas. Recall that  $B \in H_n$  is nonnegative definite if and only if its all principle minors are nonnegative. Thus we obtain.

**Lemma 3.2** *Let  $B = [b_{ij}]_{i,j=1}^n \in H_{n,+}$ . Then for each  $i \neq j \in \langle n \rangle$   $b_{ii} b_{jj} \geq |b_{ij}|^2$ . In particular, if  $b_{ii} = 0$  then  $b_{ij} = b_{ji} = 0$  for  $j = 1, \dots, n$ .*

**Lemma 3.3** *Let  $A, B \in H_{n,+}$ . Then  $AB = 0$  if and only if  $\text{Tr} AB = 0$ .*

**Proof.** Clearly, if  $AB = 0$  the  $\text{Tr } AB = 0$ . Assume that  $\text{Tr } AB = 0$ . As above we may assume that  $A$  is a diagonal matrix of the form (2.4) and  $B = [b_{ij}]_{i,j=1}^n$ . So  $\text{Tr}(AB) = \sum_{i=1}^n a_i b_{ii}$ . Since  $B \succeq 0$  each  $b_{ii} \geq 0$ . So  $\text{Tr}(AB) = 0$  yields that  $a_i b_{ii} = 0, i = 1, \dots, n$ . Since  $a_1 \geq \dots \geq a_n \geq 0$  we deduce from Lemma 3.2 that  $A = A_1 \oplus 0_{t \times t}, B = 0_{s \times s} \oplus B_2$ , where  $A_1 \in \mathbb{H}_{s,+}, B_2 \in \mathbb{H}_{t,+}$  and  $s, t$  are nonnegative integers such that  $s + t = n$ . Clearly  $AB = 0$ .  $\square$

**Lemma 3.4** *Let  $A, B \in \mathbb{C}^{n \times n}$  and  $2 \leq k \in \mathbb{N}$ . Denote by  $T_k(A, B) \in \mathbb{C}^{kn \times kn}$  the following  $k \times k$  block bidiagonal Toeplitz matrix*

$$T_k(A, B) = \begin{bmatrix} A & B & 0 & 0 & \dots & 0 & 0 \\ 0 & A & B & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & A & B \\ 0 & 0 & 0 & 0 & \dots & 0 & A \end{bmatrix}.$$

*Then for  $m \in \mathbb{N}$   $T_k(A, B)^m$  is the following upper triangular Toeplitz matrix:*

$$\begin{bmatrix} S_{m,0}(A, B) & S_{m-1,1}(A, B) & S_{m-2,2}(A, B) & \dots & S_{m-k+2,k-2}(A, B) & S_{m-k+1,k-1}(A, B) \\ 0 & S_{m,0}(A, B) & S_{m-1,1}(A, B) & \dots & S_{m-k+3,k-3}(A, B) & S_{m-k+2,k-2}(A, B) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & S_{m,0}(A, B) & S_{m-1,1}(A, B) \\ 0 & 0 & 0 & \dots & 0 & S_{m,0}(A, B) \end{bmatrix}.$$

**Proof.** The lemma follows straightforward by induction from (2.2).

Recall the Neumann expansion

$$(I_{kn} - tT_k(A, B))^{-1} = \sum_{m=0}^{\infty} t^m T_k(A, B)^m. \quad (3.3)$$

Let

$$(I_{kn} - tT_k(A, B))^{-1} = ((I_{kn} - tT_k(A, B))_{ij}^{(-1)})_{i,j=1}^k. \quad (3.4)$$

Then Lemma 3.4 and (3.3) yield.

$$\begin{aligned} (I_{kn} - tT_k(A, B))_{1k}^{(-1)} &= \sum_{m=0}^{\infty} t^m S_{m-k+1,k-1}(A, B) = \\ &= t^{k-1} \sum_{m=k-1}^{\infty} t^{m-k+1} S_{m-k+1,k-1}(A, B). \end{aligned} \quad (3.5)$$

**Lemma 3.5** *Let  $A, B \in \mathbb{C}^{n \times n}$ . Then*

$$(I - tA)^{-1} (B(I - tA)^{-1})^{k-1} = \sum_{m=k-1}^{\infty} t^{m-k+1} S_{m-k+1,k-1}(A, B). \quad (3.6)$$

**Proof.** Observe that

$$I_{kn} - tT_k(A, B) = T_k(I - tA, -tB) = T_k(I, -tB(I - tA)^{-1})T_k(I - tA, 0).$$

Hence

$$(I_{kn} - tT_k(A, B))^{-1} = T_k(I - tA, 0)^{-1} T_k(I, -tB(I - tA)^{-1})^{-1} = T_k((I - tA)^{-1}, 0) T_k(I, -tB(I - tA)^{-1})^{-1}.$$

Observe next that for any  $C \in \mathbb{C}^{n \times n}$   $T_k(I, -C) = I_{nk} - T_k(0, C)$ , where  $T_k(0, C)$  is nilpotent. Hence  $T_k(I, -C)^{-1} = I_{kn} + \sum_{m=1}^{k-1} C^m$ . Furthermore the  $(1, k)$  block of  $T_k(I, -C)^{-1}$  is  $C^{k-1}$ . Hence the  $(1, k)$  block of  $(I_{kn} - tT_k(A, B))^{-1}$  is equal to  $t^{k-1}(I - tA)^{-1}(B(I - tA)^{-1})^{k-1}$ . Use (3.5) to deduce (3.6).  $\square$

**Corollary 3.6** *Let  $A, B \in H_{n,+}$ . Then the BMV conjecture is equivalent to the statement that for each  $k \geq 1$  the Taylor series of  $\text{Tr}(I - tA)^{-1}(B(I - tA)^{-1})^{k-1}$  are nonnegative.*

**Proof of Theorem 3.1.** The case  $\text{Tr } AB = 0$  is taken care by Lemma 3.3. Assume that  $\text{Tr } AB > 0$ . We will prove first the equality (3.2). Assume that  $A$  of the form (2.4). Then  $(I - tA)^{-1} = \text{diag}((1 - a_1 t)^{-1}, \dots, (1 - a_n t)^{-1})$ . Let  $B = [b_{ij}]_{i,j=1}^n$ . Then

$$\text{Tr}(I - tA)^{-1}(B(I - tA)^{-1})^k = \sum_{i_1=i_{k+1}, \dots, i_{k+1}=1}^n \frac{\prod_{j=1}^k b_{i_j i_{j+1}}}{\prod_{j=1}^{k+1} (1 - a_{i_j} t)}, \quad k \geq 1. \quad (3.7)$$

Assume first that  $b_{11} > 0$ , i.e. the value of  $p$  in the statement of the theorem is 1. So  $a_1 = \dots = a_l > a_{l+1}$ . Clearly the rational function given in (3.7) has poles at most at the points  $z = \frac{1}{a_i}$  for all  $i$  such that  $a_i > 0$ . We now show that the  $\frac{1}{a_1}$  is a pole of order  $k + 1$  exactly. Clearly, the coefficient of the term  $(1 - a_1 t)^{k+1}$  is obtained by letting  $i_1 = i_{k+1}, \dots, i_k$  range from 1 to  $l$ . Hence this coefficient is equal to  $\text{Tr } C^k$ , where  $C = [b_{ij}]_{i,j=1}^l$ . Since  $B \succeq 0$  it follows that  $C \succeq 0$ . Assume that  $\lambda_1(C) \geq \dots \lambda_l(C) \geq 0$ . The maximal characterization of  $\lambda_1(C)$  yields that  $\lambda_1(C) \geq b_{11}$ . Hence

$$\text{Tr } C^k = \sum_{i=1}^l \lambda_i(C)^k \geq \lambda_1(C)^k \geq b_{pp}^k > 0, \quad (3.8)$$

where  $p = 1$ . Write

$$\text{Tr}(I - tA)(B(I - tA)^{-1})^k = \frac{\text{Tr } C^k}{(1 - a_1 t)^{k+1}} + f_k(t, A, B).$$

Note that  $f_k(t, A, B)$  may have poles only at  $\frac{1}{a_i}$ . Furthermore, the order of the pole at  $\frac{1}{a_1}$  is at most  $k$ . Hence asymptotically, the contribution to the  $m$  coefficient of the power series of  $\text{Tr}(I - tA)(B(I - tA)^{-1})^k$  is from the term  $\frac{\text{Tr } C^k}{(1 - a_1 t)^{k+1}}$ . This establish the equality (3.2). Use (3.8) for  $p = 1$  to deduce (3.1) from (3.2).

Suppose now that the value of  $p$  in the theorem is greater than 1. From the arguments of the proof of Lemma 3.3 it follows that

$$A = A_1 \oplus A_2, \quad A_1 = \text{diag}(a_1, \dots, a_{p-1}), \quad A_2 = \text{diag}(a_i, \dots, a_n), \\ B = 0_{(p-1) \times (p-1)} \oplus B_2, \quad B_2 = [b_{ij}]_{i,j=p}^n.$$

Then  $\text{Tr}(I - tA)(B(I - tA)^{-1})^k = \text{Tr}(I - tA_2)(B_2(I - tA_2)^{-1})^k$  and the theorem follows from the previous discussed case.  $\square$

## 4 The case $n = k = 3$

The first nontrivial case of the BMV conjecture is is the dimension  $n = 3$ , i.e.  $3 \times 3$  matrices. The first nontrivial case  $k = 3$  is that we consider the coefficient of  $t^3$  in  $\text{Tr}(A + tB)^m$  for all  $m$  and all  $3 \times 3$  matrices nonnegative definite matrices  $A, B$ . Assume for simplicity that we deal with real symmetric matrices. Then the nontrivial case

$$B = \begin{bmatrix} x & -u & -v \\ -u & y & -w \\ -v & -w & z \end{bmatrix}, \quad u, v, w > 0. \quad (4.1)$$

It is enough to consider the case where  $A = \text{diag}(1, a, 0)$ , where  $a \in [0, 1]$  and  $\det B = 0$  and  $B$  nonnegative definite. This is equivalent to

$$2uvw = xyz - u^2z - v^2y - w^2x, \quad 0 \leq x, y, z, \quad u^2 \leq xy, \quad v^2 \leq xz, \quad w^2 \leq yz. \quad (4.2)$$

Thus we need to show that all the coefficients in Taylor series of  $\text{Tr}(I - tA)^{-1}(B(I - tA)^{-1})^3$  are all nonnegative. Clearly

$$B(I - tA)^{-1} = \begin{bmatrix} \frac{x}{1-t} & -\frac{u}{1-at} & -v \\ -\frac{u}{1-t} & \frac{y}{1-at} & -w \\ -\frac{v}{1-t} & -\frac{w}{1-at} & z \end{bmatrix}.$$

Now compute the diagonal entries of  $(B(I - tA)^{-1})^3$

$$\begin{aligned} ((B(I - tA)^{-1})^3)_{11} &= \frac{x^3}{(1-t)^3} + \frac{xu^2}{(1-t)^2(1-at)} + \frac{xv^2}{(1-t)^2} + \\ &\quad \frac{yu^2}{(1-t)(1-at)^2} + \frac{zv^2}{1-t} - \frac{2uvw}{(1-t)(1-at)}, \\ ((B(I - tA)^{-1})^3)_{22} &= \frac{y^3}{(1-at)^3} + \frac{yu^2}{(1-t)(1-at)^2} + \frac{yw^2}{(1-at)^2} + \\ &\quad \frac{xu^2}{(1-t)^2(1-at)} + \frac{zw^2}{(1-at)^2} - \frac{2uvw}{(1-t)(1-at)}, \\ ((B(I - tA)^{-1})^3)_{33} &= z^3 + \frac{zv^2}{(1-t)} + \frac{zw^2}{(1-at)} + \\ &\quad \frac{xv^2}{(1-t)^2} + \frac{yw^2}{(1-at)^2} - \frac{2uvw}{(1-t)(1-at)}. \end{aligned}$$

Hence  $\text{Tr}(I - tA)^{-1}(B(I - tA)^{-1})^3$  is

$$\begin{aligned} & \frac{1}{1-t} \left( \frac{x^3}{(1-t)^3} + \frac{xu^2}{(1-t)^2(1-at)} + \frac{xv^2}{(1-t)^2} + \right. \\ & \quad \left. \frac{yu^2}{(1-t)(1-at)^2} + \frac{zv^2}{1-t} - \frac{2uvw}{(1-t)(1-at)} \right) + \\ & \frac{1}{1-at} \left( \frac{y^3}{(1-at)^3} + \frac{yu^2}{(1-t)(1-at)^2} + \frac{yw^2}{(1-at)^2} + \right. \\ & \quad \left. \frac{xu^2}{(1-t)^2(1-at)} + \frac{zw^2}{(1-at)^2} - \frac{2uvw}{(1-t)(1-at)} \right) + \\ & \quad z^3 + \frac{zv^2}{(1-t)} + \frac{zw^2}{(1-at)} + \\ & \quad \frac{xv^2}{(1-t)^2} + \frac{yw^2}{(1-at)^2} - \frac{2uvw}{(1-t)(1-at)}. \end{aligned}$$

So one has to show that all the coefficients of these series are nonnegative under the conditions (4.2).

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